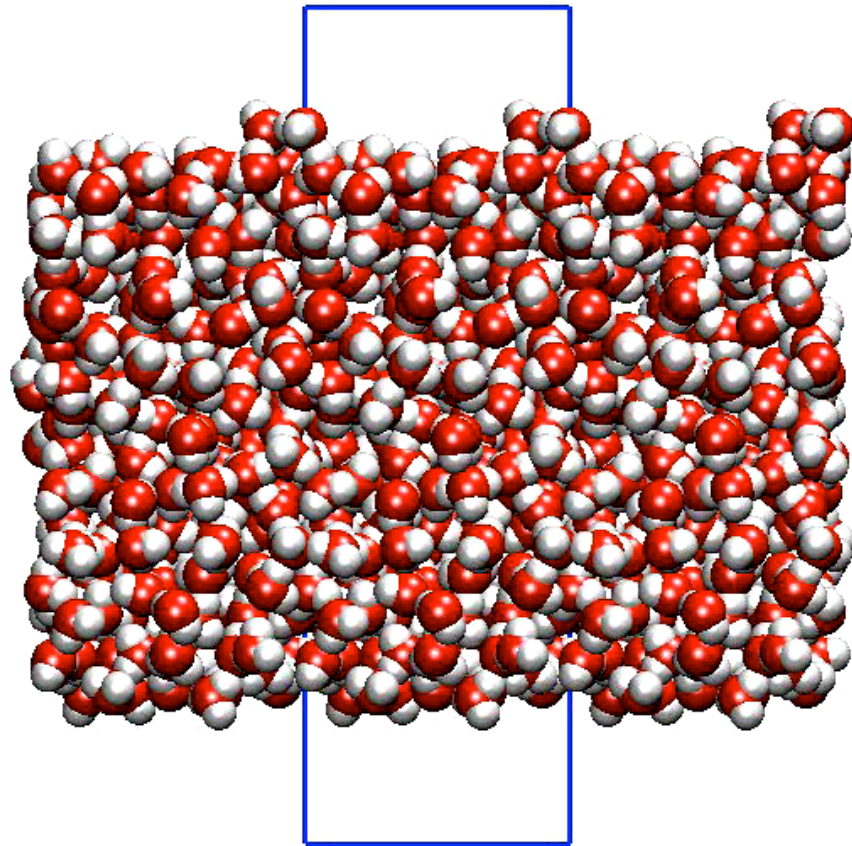


Simulation of neat water/vapor interface



This simulation was done in support of our National Security mission which requires us to understand the fate and transport of chemical/biological agents in the atmosphere. In order to demonstrate the validity of our methodology, our first goal was to study the neat water/vapor interface. This is the first stable *ab initio* water/vapor interface. The detailed structure of this interface is still an open question and an area of active research. Simulations of this magnitude are *necessary* and require the dedicated use of the MCR cluster in order to elucidate the precise orientation of the molecular dipole moment of water at the interface.